Advancements in Large-Scale Simulation of Microscale Porous Medium Systems Using Lattice Boltzmann Methods

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Introduction

Microscale modeling of porous medium systems has matured as an important tool for not only advancing fundamental mechanistic understanding of flow and transport phenomena but also for closing, evaluating, and validating a new generation of high-fidelity macroscale models. To support these dual objectives, we target the simulation of systems that are highly resolved and sufficiently large to ensure a representative elementary volume, which can lead to state spaces with 10^{10} unknowns in space and order 10^8 time steps. The scale of these desired simulations presents significant computational challenges that impact the choice of methods, algorithms, and computational platform. The goal of this work is to illustrate approaches that make such simulations feasible, compare alternative approaches, and provide examples and uses of such large-scale simulations.

Methods

We detail a D3Q19 lattice-Boltzmann method (LBM) approach based upon a color model, level-set methods to resolve interfaces, and *in situ* analysis tools [1]to upscale simulation results to the macroscale while limiting data movement. A common LBM structure is detailed, streaming algorithms [2, 3] are compared, communication and load balancing issues addressed, efficiency on modern high-performance computing architectures assessed, and weak and strong scaling evaluated for some of the largest LBM simulations ever reported. The specific physics considered includes single and two-fluid phase flow for both Newtonian and non-Newtonian fluids. Evolving work on adaptive methods [4] and more challenging processes is also discussed.

Results

We compare a new flux boundary condition used to aid in the accurate simulation of drainage and imbibition of multiphase Newtonian flow and the flow of a single non-Newtonian fluid to standard pressure boundary conditions. We demonstrate the importance of the streaming algorithm for achieving a high fraction of theoretical peak performance on a new supercomputing hybrid-node architecture. With a load-balanced adaptive algorithm aimed at focusing comutational resources on the active domain of two-fluid-phase flow simulations, such as shown in Figure 1, we show that we can achieve a 10-fold decrease in time-to-solution.

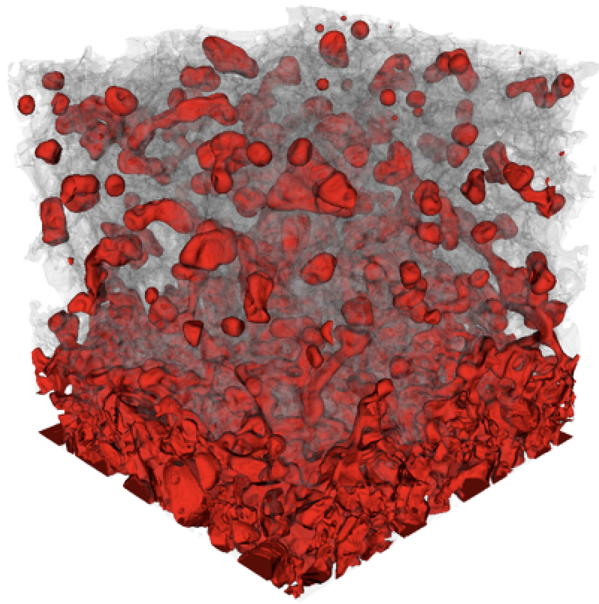

Figure 1: Simulation of a two-fluid-phase porous media system. Fluid trapped during imbitition illustrated by reduced opacity of the second fluid.

References

[1] J. E. McClure, M. A. Berrill, J. F. Prins, and C. T. Miller. Asynchronous in situ connected-components analysis for complex fluid flows. In *2016 Second Workshop on In Situ Infrastructures for Enabling Extreme-Scale Analysis and Visualization (ISAV)*, pages 12–17, Nov 2016.

[2] Peter Bailey, Joe Myre, Stuart D. C. Walsh, David J. Lilja, and Martin O. Saar. Accelerating lattice Boltzmann fluid flow simulations using graphics processors. In *Proceedings of the 2009 International Conference on Parallel Processing*, ICPP '09, pages 550–557, Washington, DC, USA, 2009. IEEE Computer Society.

[3] J.E. McClure, J.F. Prins, and C.T. Miller. A novel heterogeneous algorithm to simulate multiphase flow in porous media on multicore CPU-GPU systems. *Computer Physics Communications*, 185(7):1865 – 1874, 2014.

[4] Amanda L. Dye, James E. McClure, David Adalsteinsson, and Cass T. Miller. An adaptive lattice Boltzmann scheme for modeling two-fluid-phase flow in porous medium systems. *Water Resources Research*, 52(4):2601–2617, 2016.